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Production Rates for Electron Beams and Swarms in Nitrogen

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Detailed calculations of the deposition of electron energy in molecular nitrogen are presented. Two cases are considered. In the first one, the electrons are accelerated by a constant, uniform electric field as in a swarm experiment. The reduced electric field strength ranges from 1 to 300 Townsends. In the second case, deposition is initiated by electron beams with energies up to 10 MeV. Production rates for the various excitation channels are given. Keywords: Ion pairs, Electron swarms, Molecular Rotation, Molecular Vibration, Cross ..., Excitation Collisions (AW)

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CONTENTS

PRODUCTION RATES FOR ELECTRON BEAMS AND SWARMS IN NITROGEN

1. Introduction

The deposition of electron energy in nitrogen is of interest in many different fields, e.g., electron beam propagation in the atmosphere, stopping of auroral electrons, electron-beam-pumped lasers. To solve this problem the cross sections for all relevant electron-atom and electron-molecule collision processes must be known. These cross sections are then incorporated into the Boltzmann equation, from which the electron distribution function is obtained. Once the distribution function is found, production rates for various processes are calculated. This report provides additional details which were not included in a previous publication[1] (denoted I) on the application of the deposition model[2-4] to nitrogen.

The form of the Boltzmann equation needed to solve the energy deposition problem and the nitrogen cross sections are summarized in Secs. 2 and 3. Section 4 contains theoretical results for electron swarms in nitrogen. For applied fields ranging from 1 - 300 Td (1 Townsend = 10^{-17} ev-cm^2), the drift velocity, characteristic energy, and production rates for the various processes are given. The fraction of energy going into different channels is shown. Results are compared with those obtained by assuming a Maxwellian electron distribution function. Section 5 gives beam deposition results where the beam electric field is ignored and the beam energy is varied. The energy expended per electron-ion pair, W, is presented, along with production rates. Finally, results are compared with those which assume the beam electrons are completely stopped.

Manuscript approved January 4, 1990.

2. Boltzmann Equation

The secondary electron distribution function is given by[1-5]

$$\frac{\partial f}{\partial t}(T,t) = N \left\{ \sum_j \left[\sigma_j\left(T+E_j\right) v\left(T+E_j\right) f\left(T+E_j,t\right) \right.\right.$$

$$\left. - \sigma_j(T)\, v(T)\, f(T,t) \right] + \sum_i \left[\int_{T+I_i}^{2T+I_i} d\varepsilon\, \sigma_i'\left(\varepsilon,\varepsilon-I_i-T\right) v(\varepsilon)\, f(\varepsilon,t) \right.$$

$$\left.\left. + \int_{2T+I_i}^{T_m} d\varepsilon\, \sigma_i'(\varepsilon,T)\, v(\varepsilon)\, f(\varepsilon,t) - \sigma_i(T)\, v(T)\, f(T,t) \right] \right\}$$

$$+ S(T,t) - \frac{\partial D}{\partial T}(T,t) - \frac{\partial H}{\partial T}(T,t) \quad , \qquad (1)$$

where $f(T,t)$ is the secondary electron density per unit energy ($cm^{-3}\ eV^{-1}$) for electrons with kinetic energy T and speed $v(T)$, T_m the maximum secondary electron energy, and N the density of the molecules which is assumed constant for the times of interest. Populations of the excited states are negligible. Equation (1) includes energy loss by electrons to all excitations with a cross section of $\sigma_j(T)$ and an excitation threshold of E_j, as well as to ionization, where $\sigma_i(T)$ is the total ionization cross section of N_2 resulting in the i-th ionization continuum and $\sigma_i'(\varepsilon,T)$ is the differential ionization cross section.

In Eq. (1), $S(T,t)$ is the source term for the generation of electrons with energy T by the beam electrons. It is assumed that the high energy primaries leave the volume of interest after at most one collision and

$$S(T,t) = N\, N_b(t)\, v(T_b) \sum_i \sigma_i'\left(T_b,T\right) \quad , \qquad (2)$$

where $N_b(t)$ is the electron density of a beam whose energy is T_b and the summation is over all ionization channels.

The term $D(T,t)$ in Eq. (1) represents the flux of the secondary electrons driven by the beam-induced electric field and is given by

$$D(T,t) = \frac{2Ne^2(E_0/N)^2 T^{1.5}\left(1+\frac{T}{2mc^2}\right)^{1.5}}{3m(\nu_m/N)\left(1+\frac{T}{mc^2}\right)} \frac{\partial}{\partial T} \frac{f(T,t)}{T^{0.5}\left(1+\frac{T}{2mc^2}\right)^{0.5}\left(1+\frac{T}{mc^2}\right)} \quad , \qquad (3)$$

where ν_m is the electron collision frequency for momentum transfer and E_0 the electric field strength. The elastic collision term, H(T,t), is

$$H(T,t) = \frac{2mN\nu_m}{M}\left[f(T,t)\left(0.5T_g - T\right) - T_g T\frac{\partial f(T,t)}{\partial T}\right] , \qquad (4)$$

where M is the mass of the target and T_g is the target temperature (in eV). For the problems considered in this paper, $\partial H/\partial T$ is small compared to the other terms in Eq. (1).

3. Cross Sections

The model consists of one effective rotational cross section, eight vibrational excitation cross sections, six triplet excitations, four singlet excitations, eleven channels leading to pure dissociation, four dissociative ionization channels, three pure ionization channels, inner-shell ionization and excitation cross sections. The momentum transfer cross section is also included. A discussion of these cross sections with references to their measurements is contained in I. Figure 1 shows the total cross sections for these processes. From these, the loss function is easily obtained and given in Fig. 2.

4. Electron Swarm Results

To simulate an electron swarm, the beam source in Eq. (1) was set to zero, some seed electrons were assumed, and a constant electric field was applied until an equilibrium was reached. If the field is high enough, equilibrium is one in which the distribution function grows at a steady exponential rate in time because of ionization. The range of fields tested was from 1 - 300 Td. For lower fields the results are sensitive to the details of the rotational cross sections and for the higher fields the two-term approximation of the Boltzmann equation becomes less accurate. For the swarm results, the background gas temperature is $T_g = 0.025$ eV.

Figure 3 gives the normalized ($\int f(\varepsilon)d\varepsilon = 1 cm^{-3}$) distribution function for several values of the reduced electric field strength, E/N (where N is the density of the neutrals). Figure 4 shows the calculated drift velocity v_d as a function of E/N. Figure 5 gives the characteristic energy ε_c and average energy ε_{ave} of the electron distribution function. To compare the results with those obtained by assuming a Maxwellian distribution, the average electron energy is used to provide a

temperature, $T_e = 2/3\varepsilon_{ave}$, for the Maxwellian. Figure 6 plots the ionization and pure dissociation coefficients. These results compare well with experimental measurements as shown in I.

Figure 7 shows the average collision frequency for momentum transfer. This collision frequency was obtained in two different ways. First, $\nu_\sigma \equiv eE/mv_d$, where v_d is the drift velocity. This is the proper average to use in the calculation of the conductivity, $\sigma = e^2 n_e/m\nu_\sigma$. Second, $\nu_{mave} \equiv \int f(\varepsilon)\sigma_m(\varepsilon)v d\varepsilon$. Also shown on the graph is the average momentum transfer collision frequency, ν^M_{mave}, calculated with f given by a Maxwellian with the same total energy.

Figure 8 gives the fraction of the energy deposited by the field in the various processes. Vibrational excitation accounts for the majority of absorption until about 100 Td where excitation of the triplet states begins to dominate.

Figure 9 gives the production rates (#/cm^3-sec) for many of the species in the model.

Finally, Fig. 10 compares the distribution function and several of the production rates with those assuming a Maxwellian of the same energy. The assumption of a Maxwellian distribution tends to underestimate triplet production, but overestimate ionization. Newman and DeTemple[6] have shown similar results.

5. Electron Beam Deposition Results

For these studies the electric field is turned off and the beam source term S(T,t), given in Eq. (2), is applied. For energies above the lowest threshold, the distribution function comes to an equilibrium.[1-3] Figure 11 shows W, the amount of energy expended by the beam in order to produce an electron-ion pair, as the beam energy is varied. W is nearly independent of beam energy for energies above a few kilovolts. Also shown in Fig. 11 are the values of W obtained by assuming the source term is a delta function at a fixed energy; this corresponds to a completely-stopped beam electron. This assumption is more accurate at lower energies.[1-4,7]

Figure 12 gives the normalized equilibrium distribution function for a 1 MeV beam and Fig. 13 shows the energy deposited per electron-ion pair in the various channels. Finally, Fig. 14 shows the production rates, in terms of the number of events per electron-ion pair, for many of the processes in the model.

6. Summary

Electron interaction with molecular nitrogen has been studied for 1) electrons which are accelerated by a constant, uniform electric field and 2) high-energy beam electrons. Details of the electron energy deposition are given.

Acknowledgment

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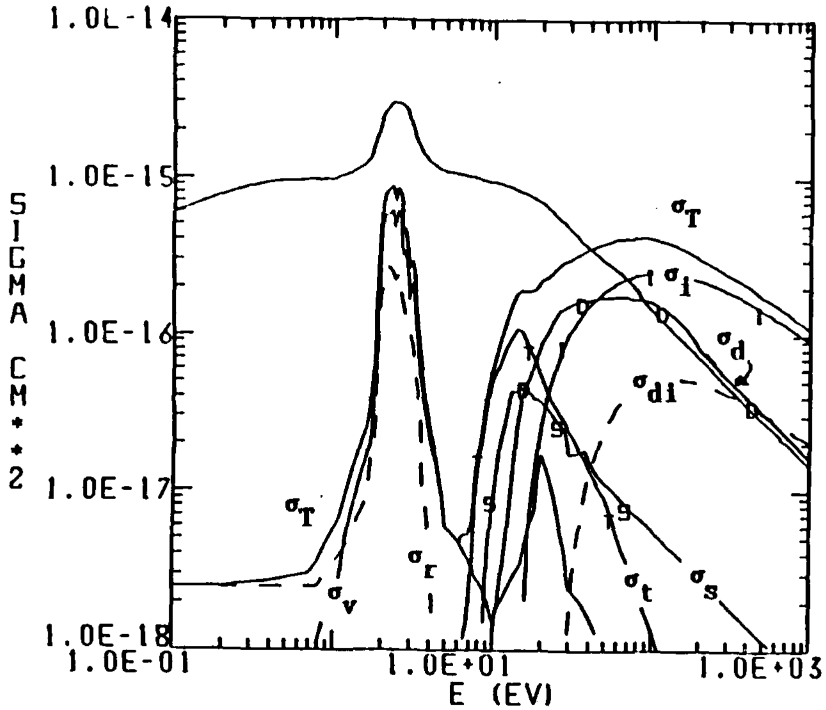

Figure 1. Nitrogen cross sections used in the model. σ_m = momentum transfer. σ_T = total inelastic. σ_i = ionization. σ_d = dissociation. σ_{di} = dissociative ioniz. (dashed). σ_s = singlet excitation. σ_t = triplet excit. σ_v = vibrational excit. σ_r = rotational excit.

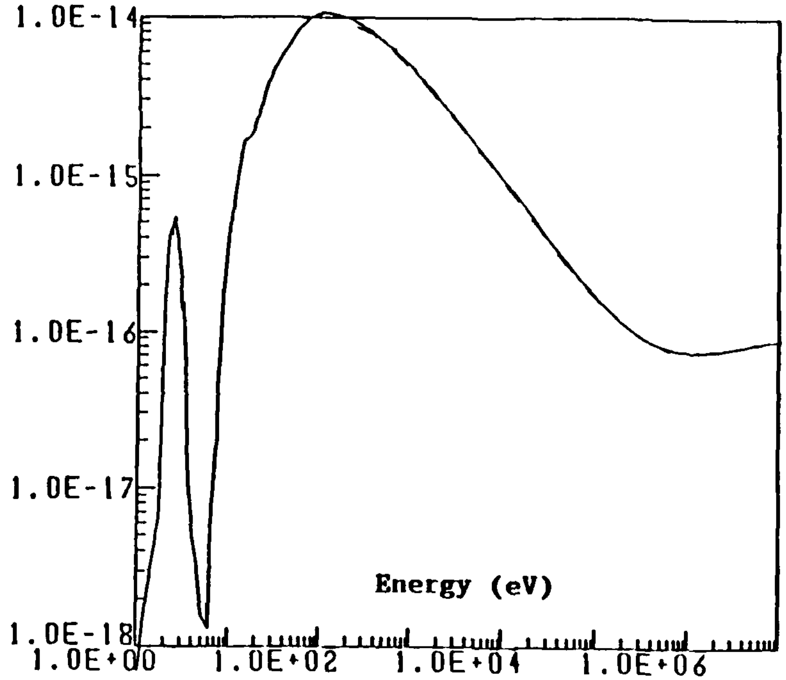

Figure 2. Loss function (eV-cm^2) in nitrogen.

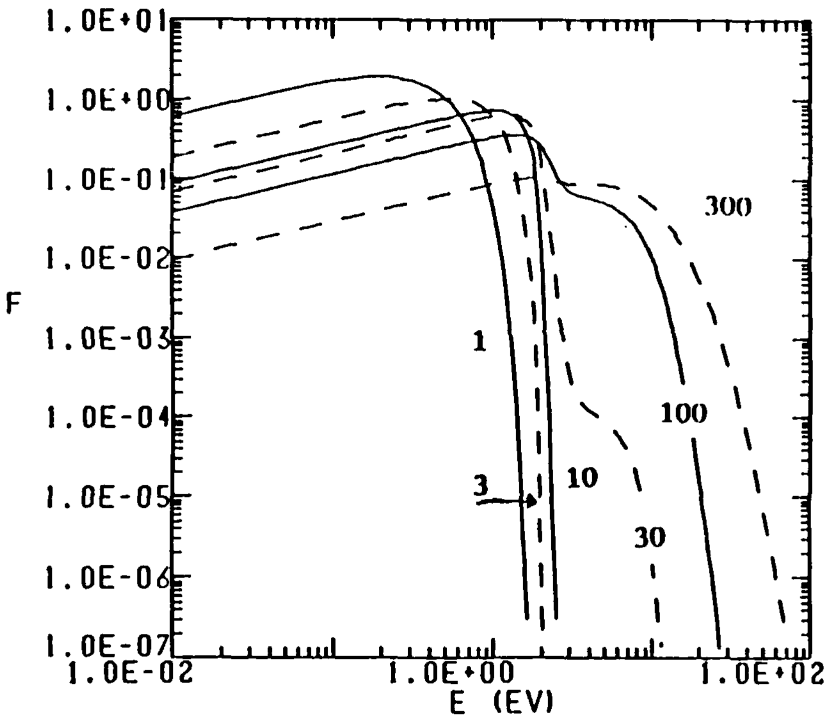

Figure 3. Normalized distribution function for reduced field strengths E/N = 1,3,10,30, 100,300 Td.

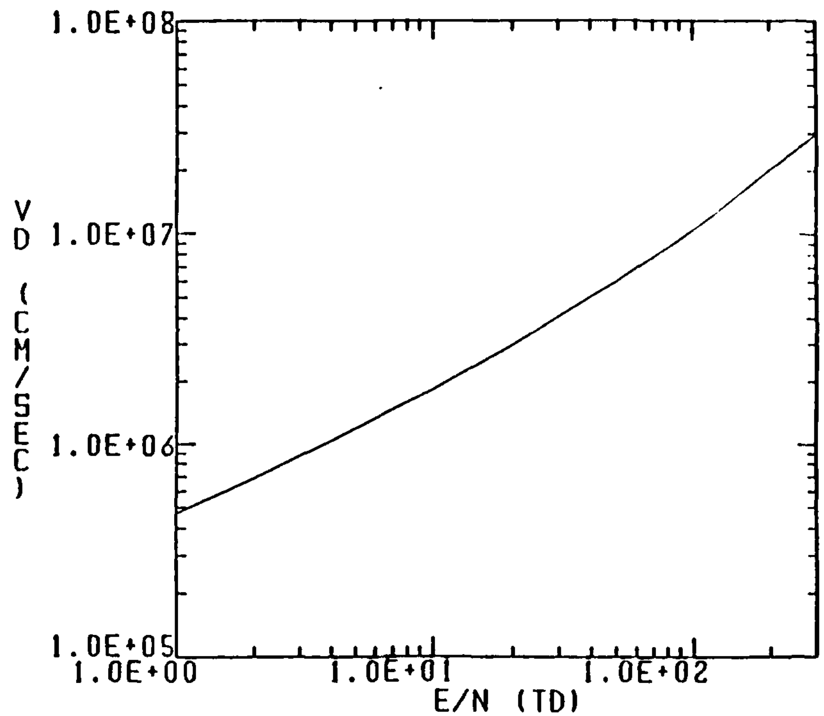

Figure 4. Calculated drift velocity (cm/sec).

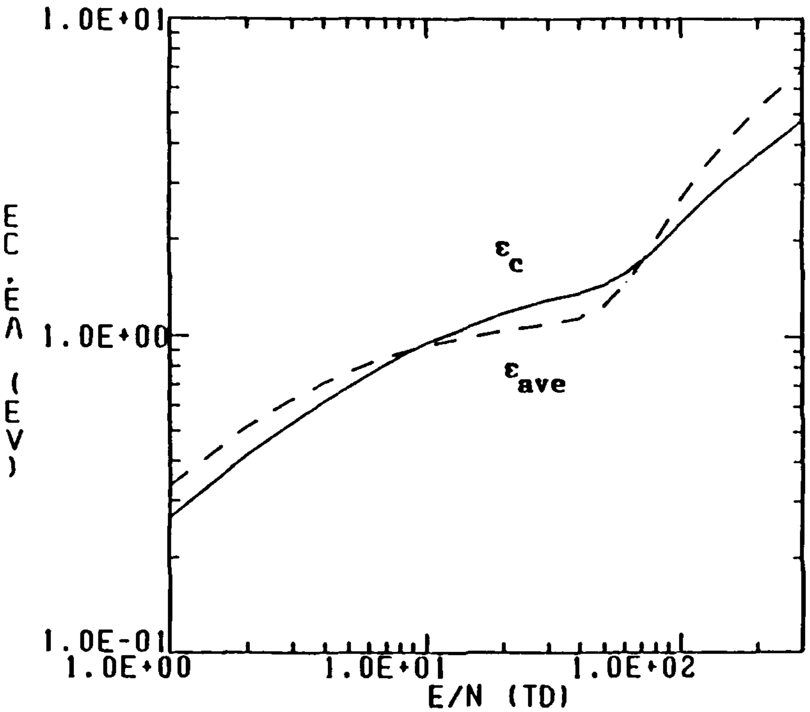

Figure 5. Calculated characteristic energy ε_c (eV) and average energy ε_{ave} (eV) of the electron distribution function.

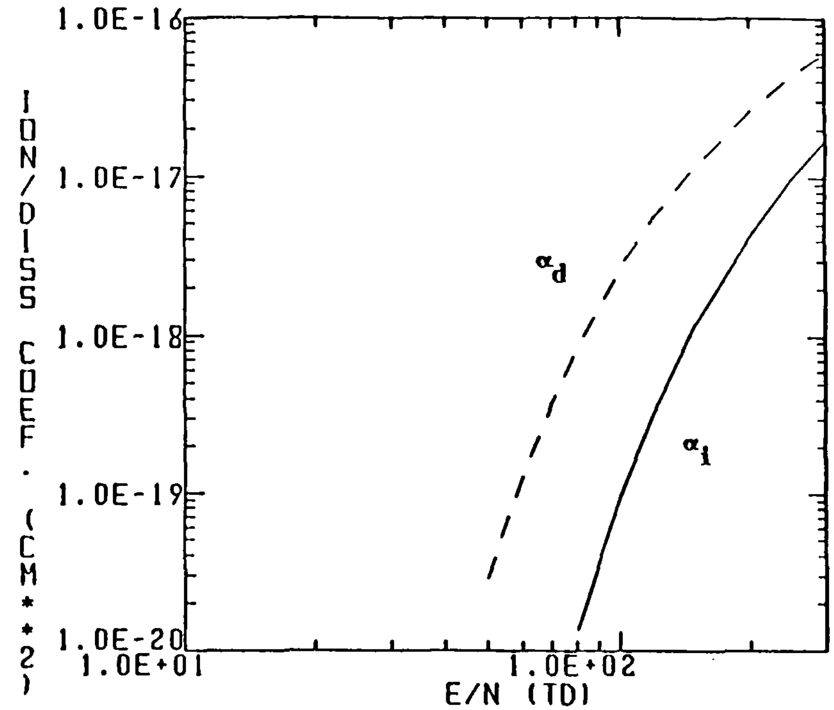

Figure 6. Ionization α_i and dissociation α_d coefficients (cm^2).

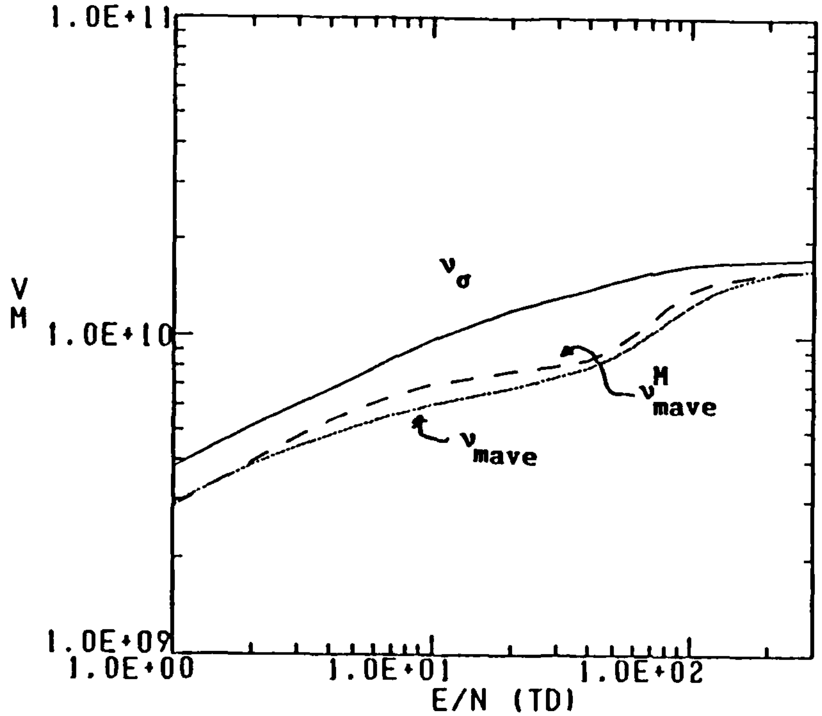

Figure 7. Various average collision frequencies (1/sec) (see text).

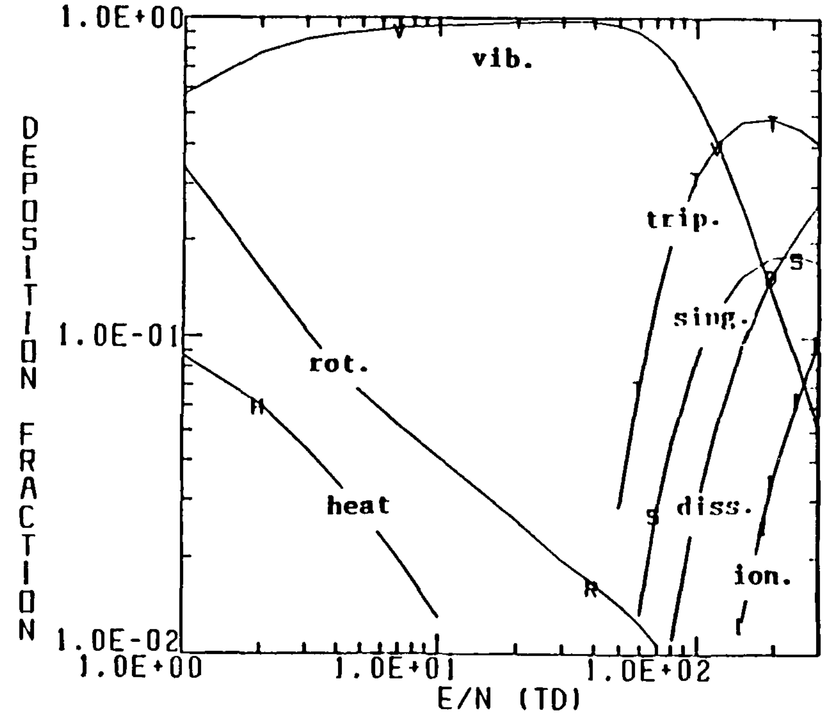

Figure 8. Fraction of energy going into different processes.

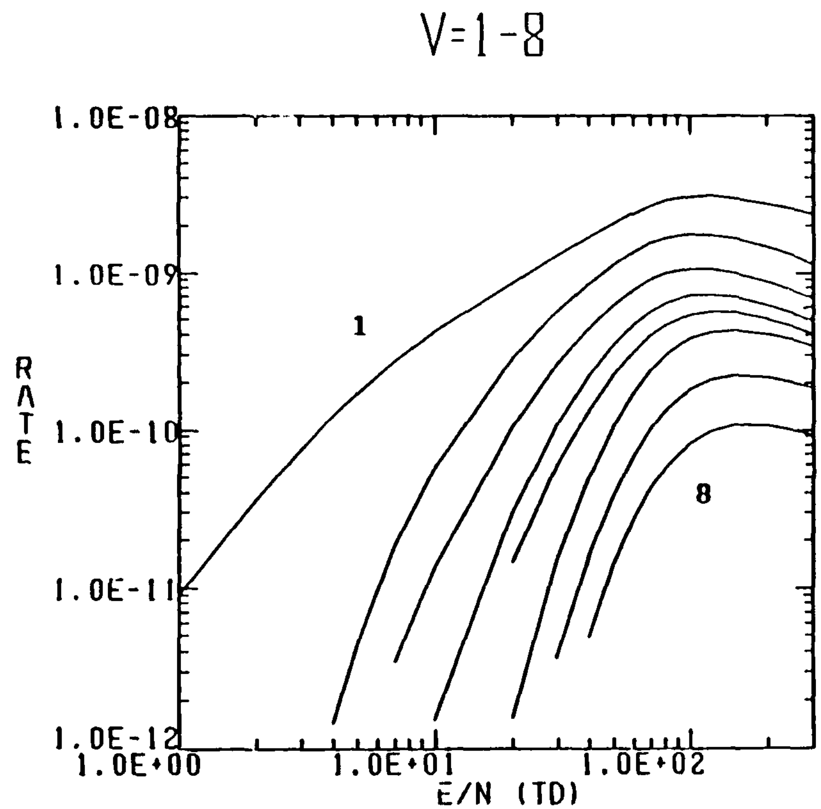

Figure 9a. Production rates (#/cm^3-sec) for excitation of vibrational levels 1-8.

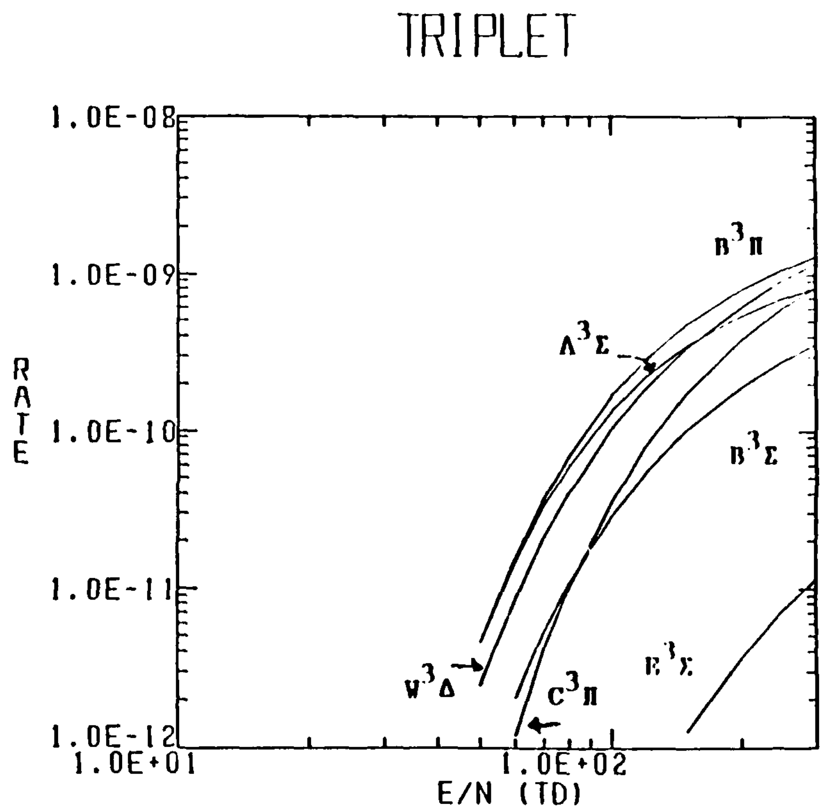

Figure 9b. Production rates (#/cm^3-sec) for triplet excitation.

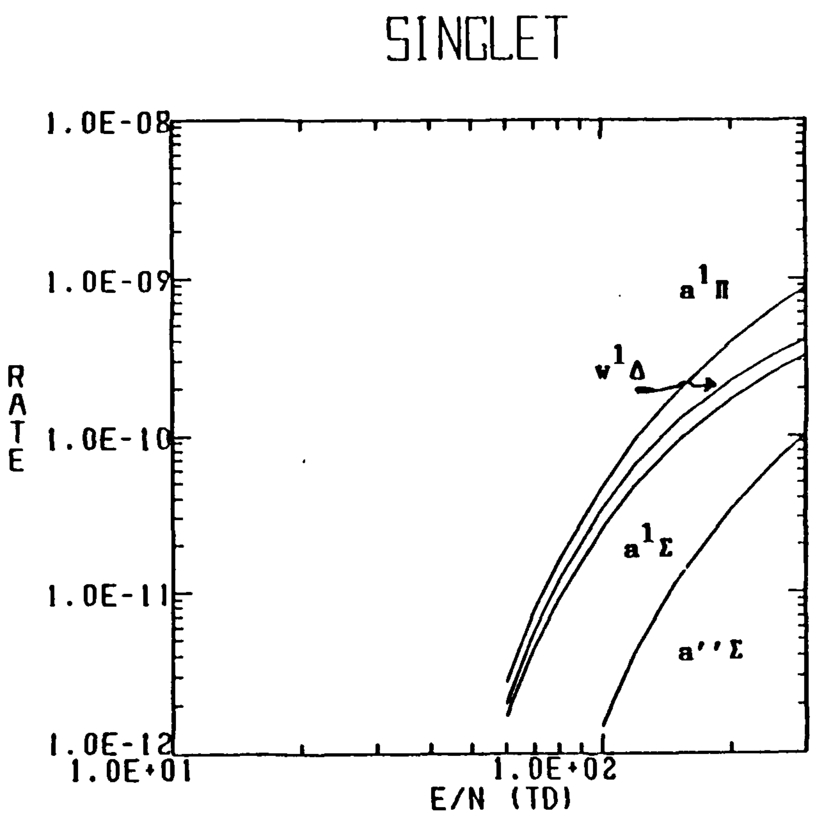

Figure 9c. Production rates ($\#/cm^3$-sec) for singlet excitation.

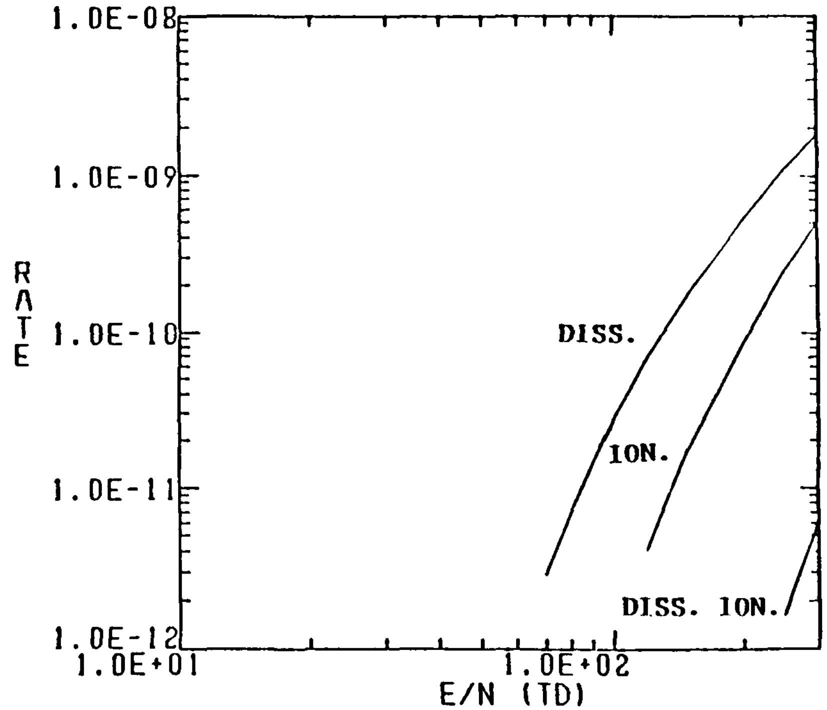

Figure 9d. Production rates ($\#/cm^3$-sec) for pure dissociation, pure ionization and dissociative ionization.

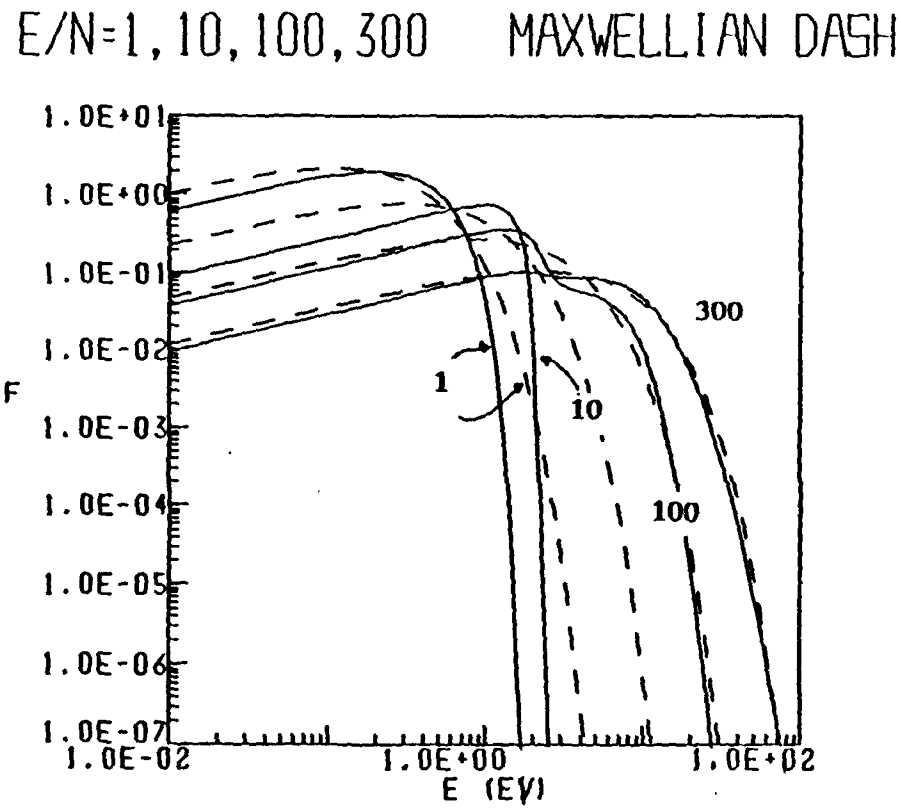

Figure 10a. Normalized distribution function and Maxwellian with the same energy (dashed) for E/N = 1,10,100,300 Td.

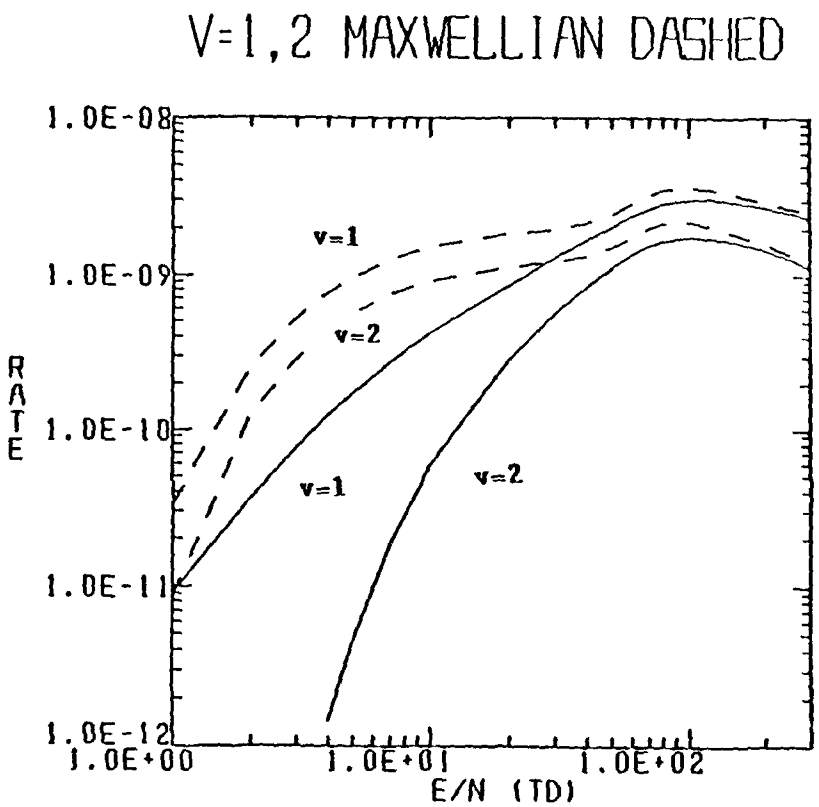

Figure 10b. Production rates (#/cm^3-sec) for excitation to the first two vibration levels for the calculated and corresponding Maxwellian (dashed) distributions.

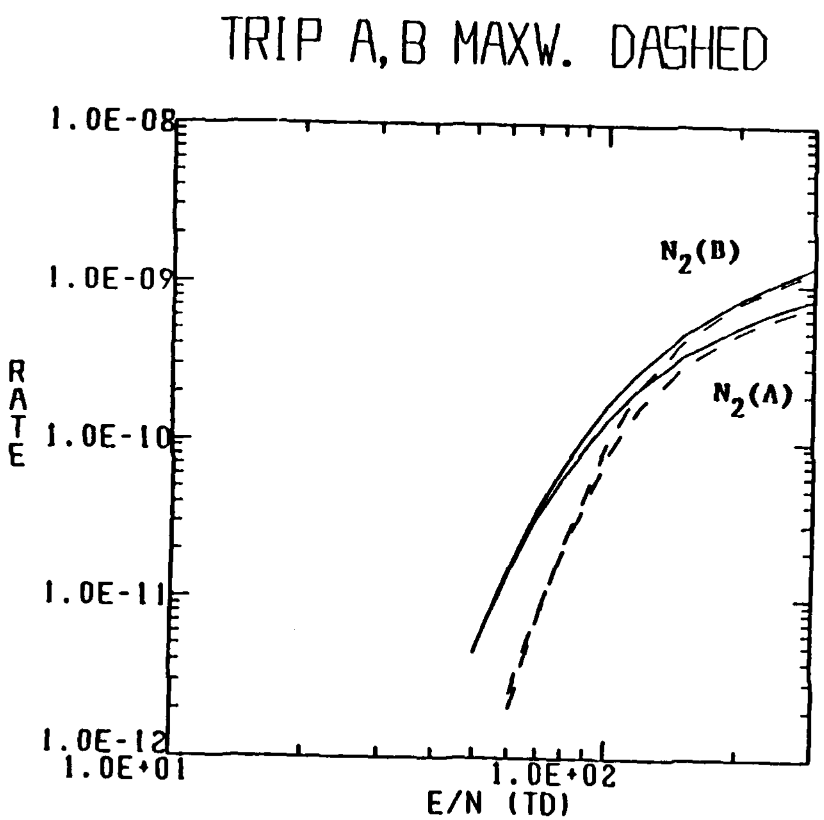

Figure 10c. Production rates (#/cm^3-sec) for the triplet A and B excitations for the calculated and corresponding Maxwellian (dashed) distributions.

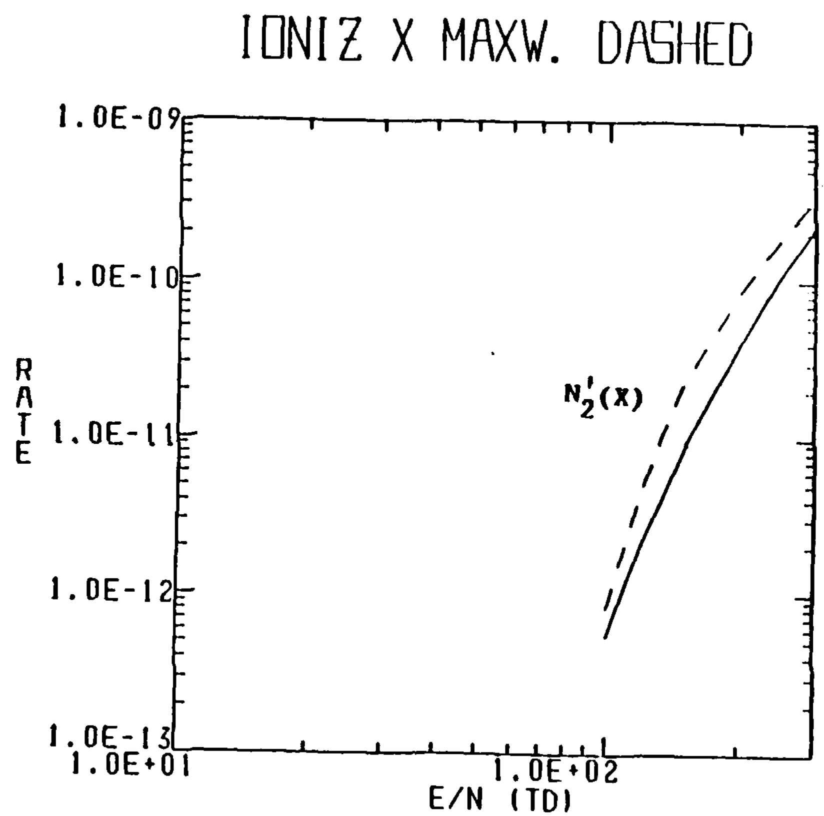

Figure 10d. Production rates (#/cm^3-sec) for the ionization state $N_2^+(X)$ for the calculated and corresponding Maxwellian (dashed) distributions.

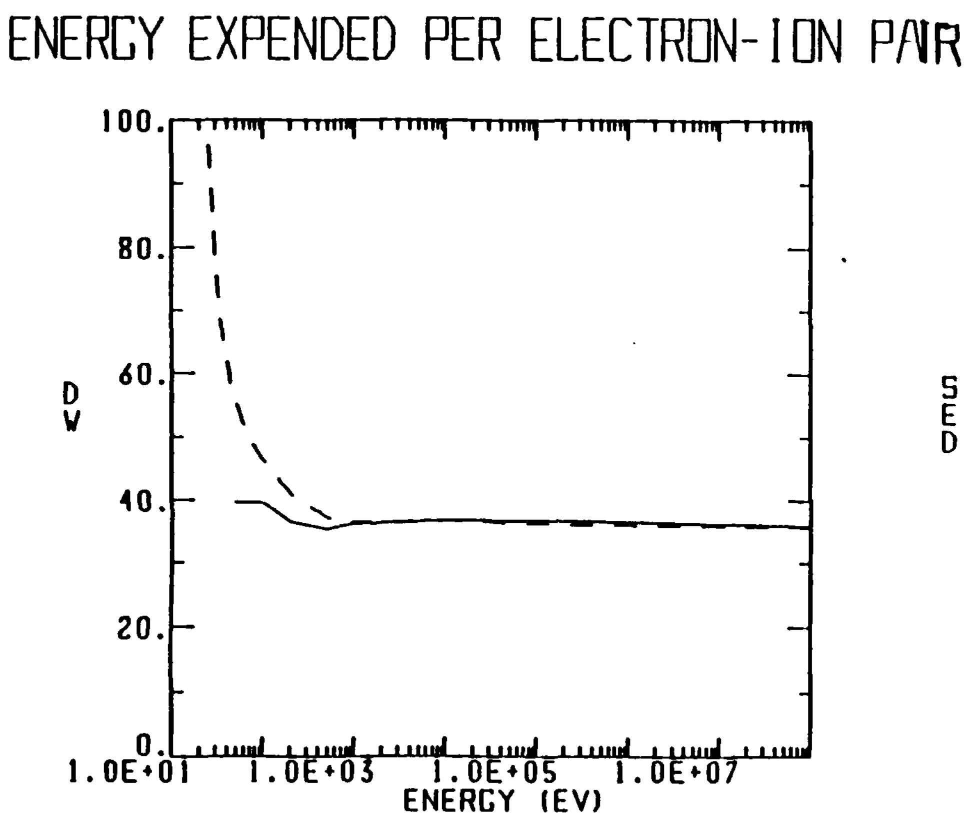

Figure 11. Energy (eV) expended per electron-ion pair for a beam source (solid) and a completely stopped source (dashed).

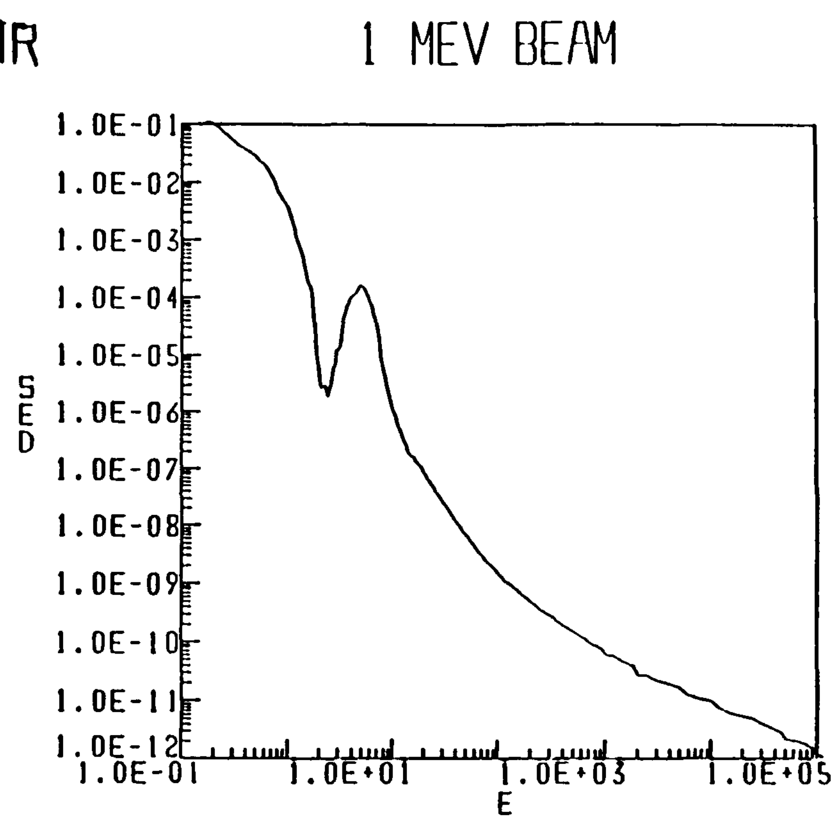

Figure 12. Equilibrium electron distribution function for a 1 MeV beam.

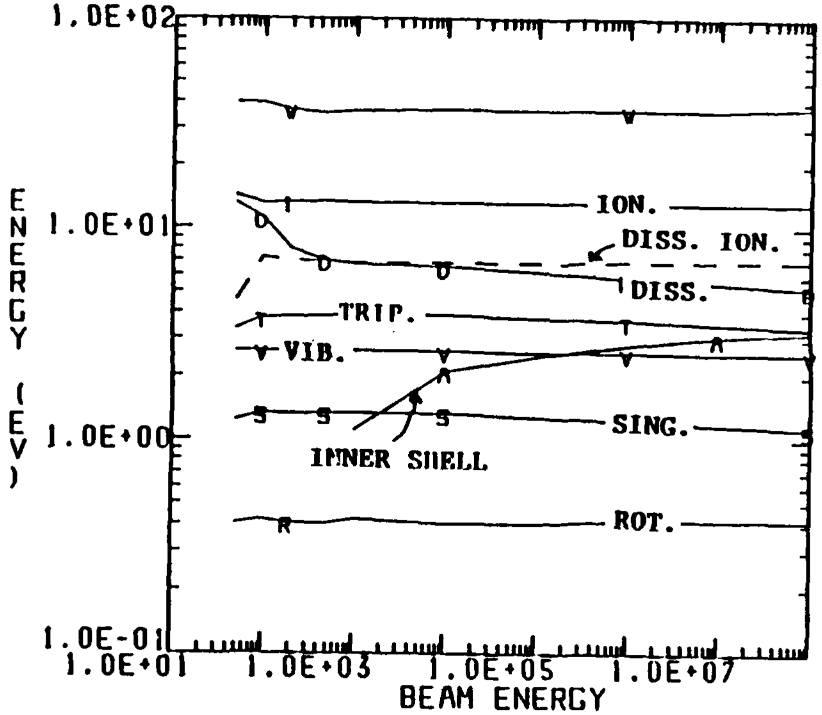

Figure 13. Energy distribution per electron-ion pair into various channels.

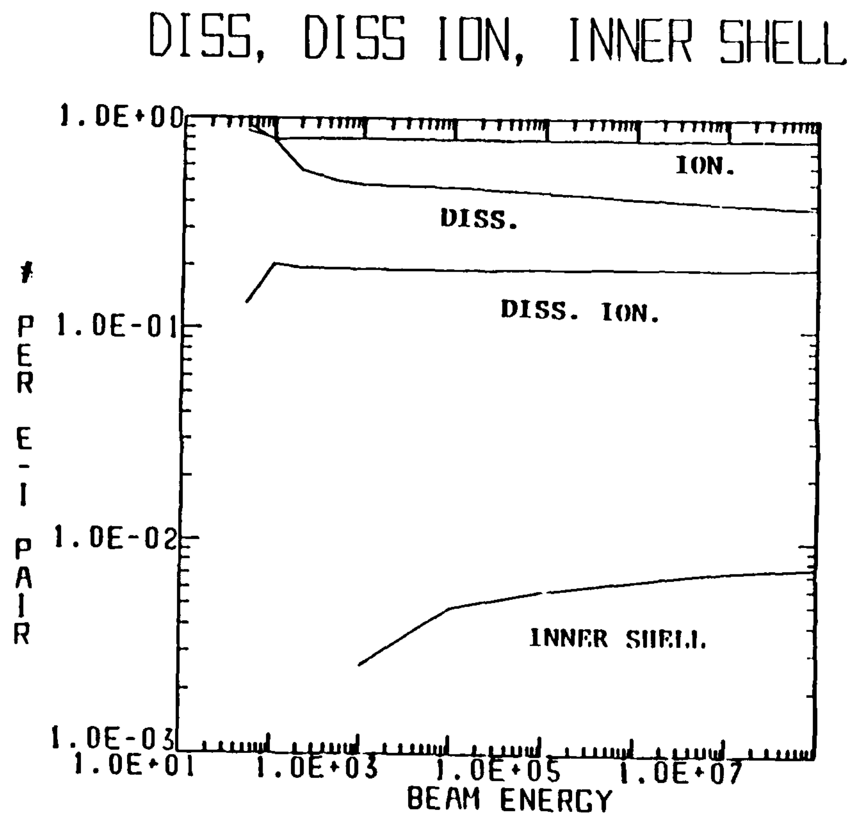

Figure 14a. Production rates (#/electron-ion pair) for pure ionization, pure dissociation, dissociative ionization and inner shell processes.

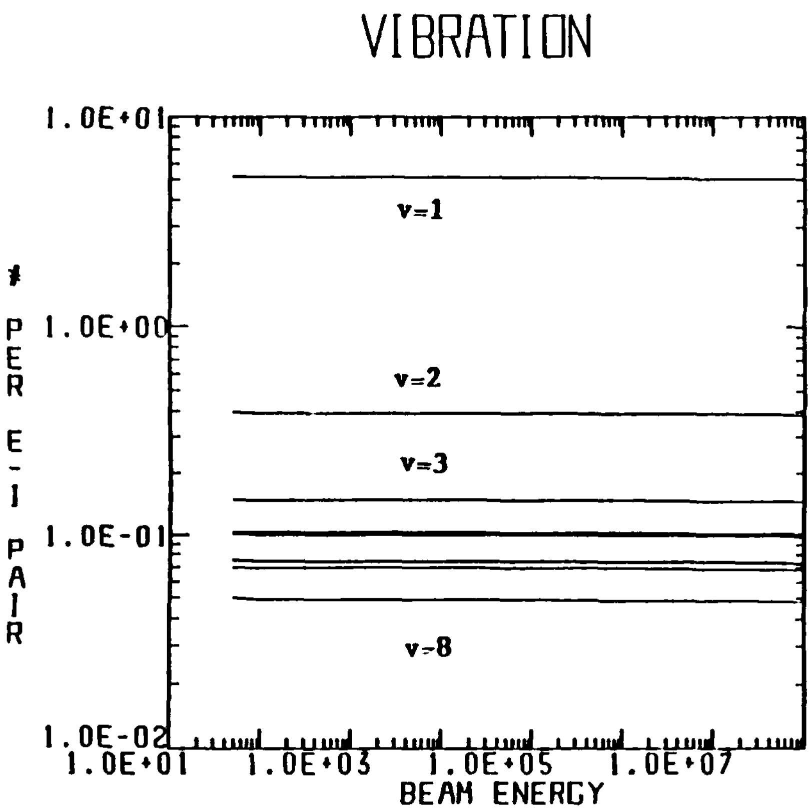

Figure 14b. Production rates (#/electron-ion pair) for vibrational excitation to levels 1-8.

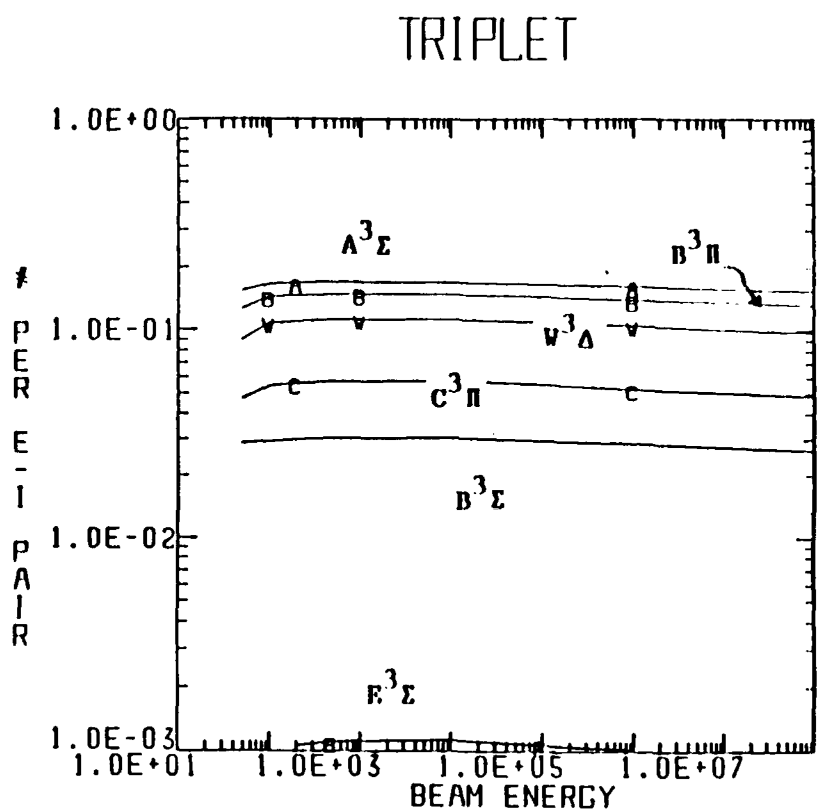

Figure 14c. Production rates (#/electron-ion pair) for triplet excitation.

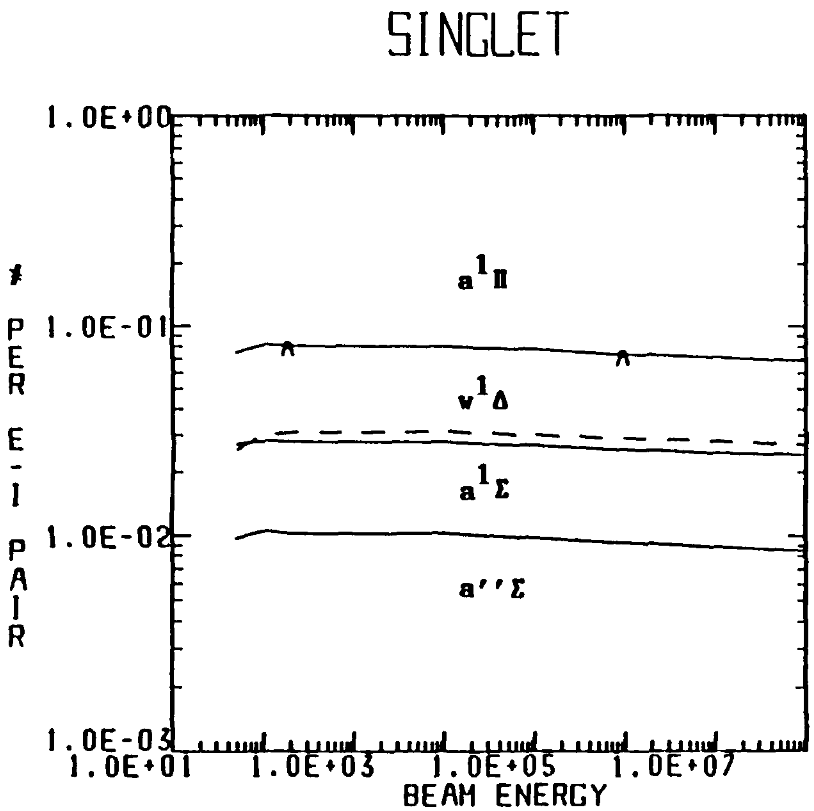

Figure 14d. Production rates (#/electron-ion pair) for singlet excitation.

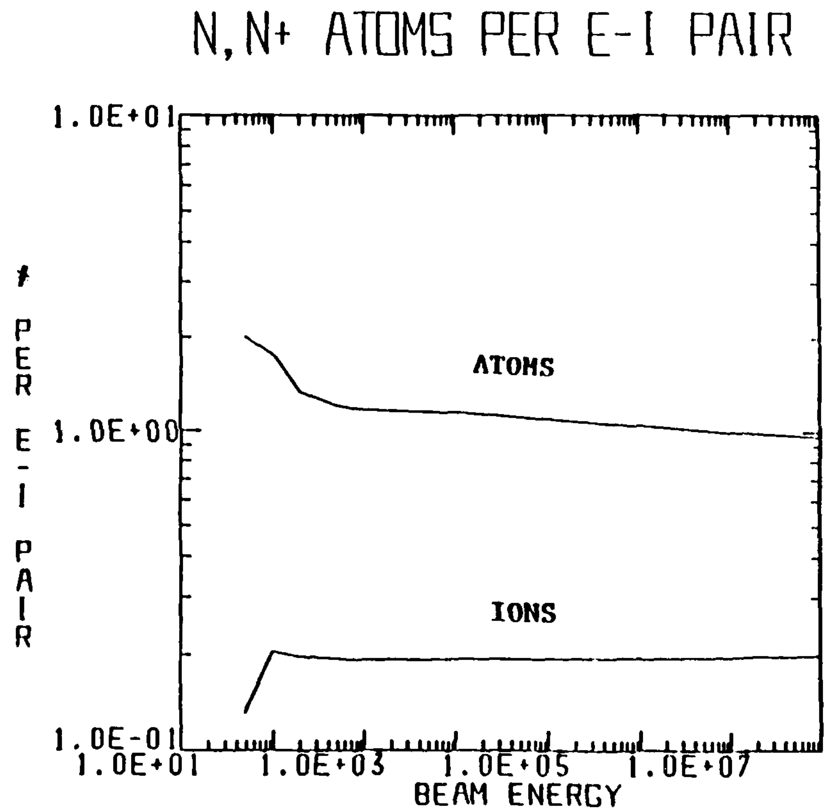

Figure 14e. Number of neutral nitrogen atoms and atomic ions produced per electron ion pair.

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